Classification of topological quantum matter with reflection symmetries

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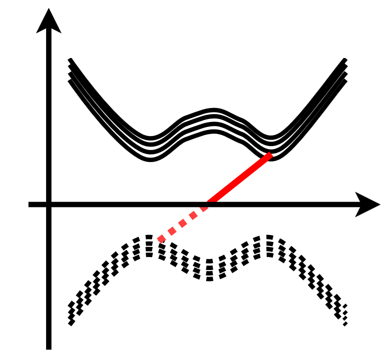
June 14th, 2016

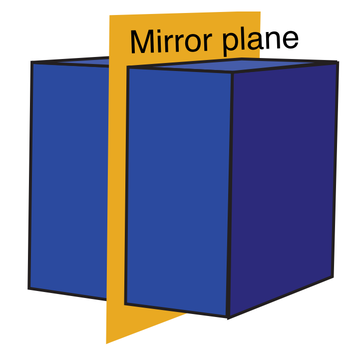
SPICE Workshop on New Paradigms in Dirac-Weyl Nanoelectronics

Outline

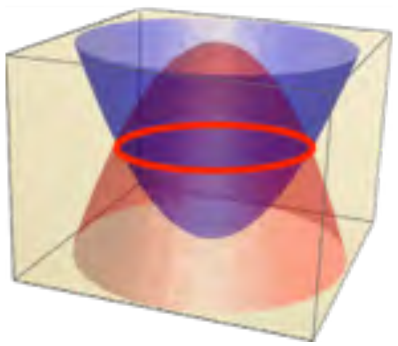
0. Introduction: Topological band theory



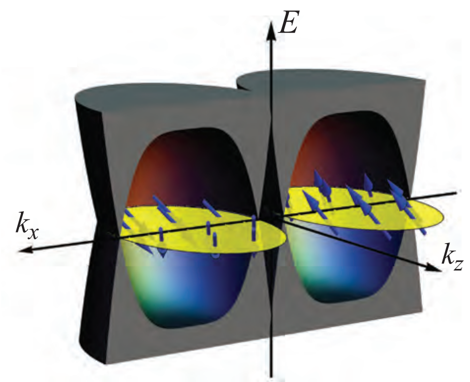
1. Topological insulators with reflection symmetry
   - Ca_3PbO, Sr_3PbO, Ba_3PbO **arXiv:1606.03456**



2. Topological nodal line semi-metals
   - Ca_3P_2, ZrSiS **PRB 93, 205132 (2016)**



3. Nodal non-centrosymmetric superconductors
   - $CePt_3Si$



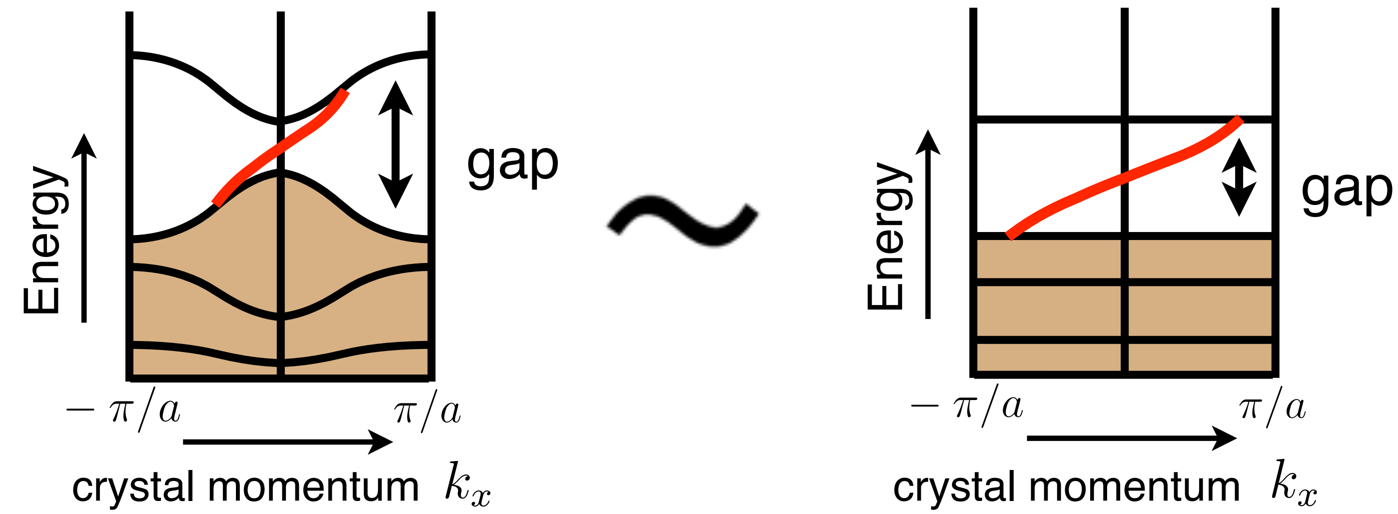
4. Conclusions & Outlook

Review articles: arXiv:1505.03535; J. Phys.: Condens. Matter 27, 243201 (2015)

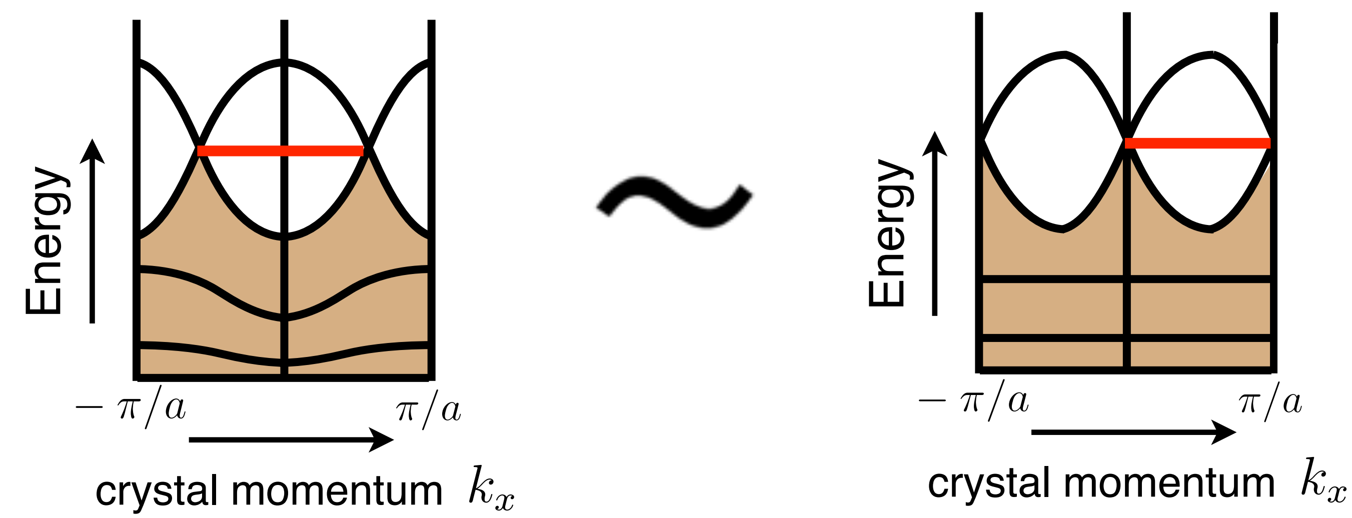
Topological band theory

- Consider band structure: $H(\boldsymbol{k}) \left| u_n(\boldsymbol{k}) \right\rangle = E_n(\boldsymbol{k}) \left| u_n(\boldsymbol{k}) \right\rangle$

- **(i) Topological equivalence for insulators (superconductors):**



- **(ii) Topological equivalence for band crossings (nodes in SCs):**



▷ symmetries to consider: *time-reversal symmetry, particle-hole, reflection*

▷ top. equivalence classes distinguished by: $n_{\mathbb{Z}} = \frac{i}{2\pi} \int_{\text{filled states}} \mathcal{F}\, d\mathbf{k} \in \mathbb{Z}$

topological invariant

- **Bulk-boundary correspondence:**

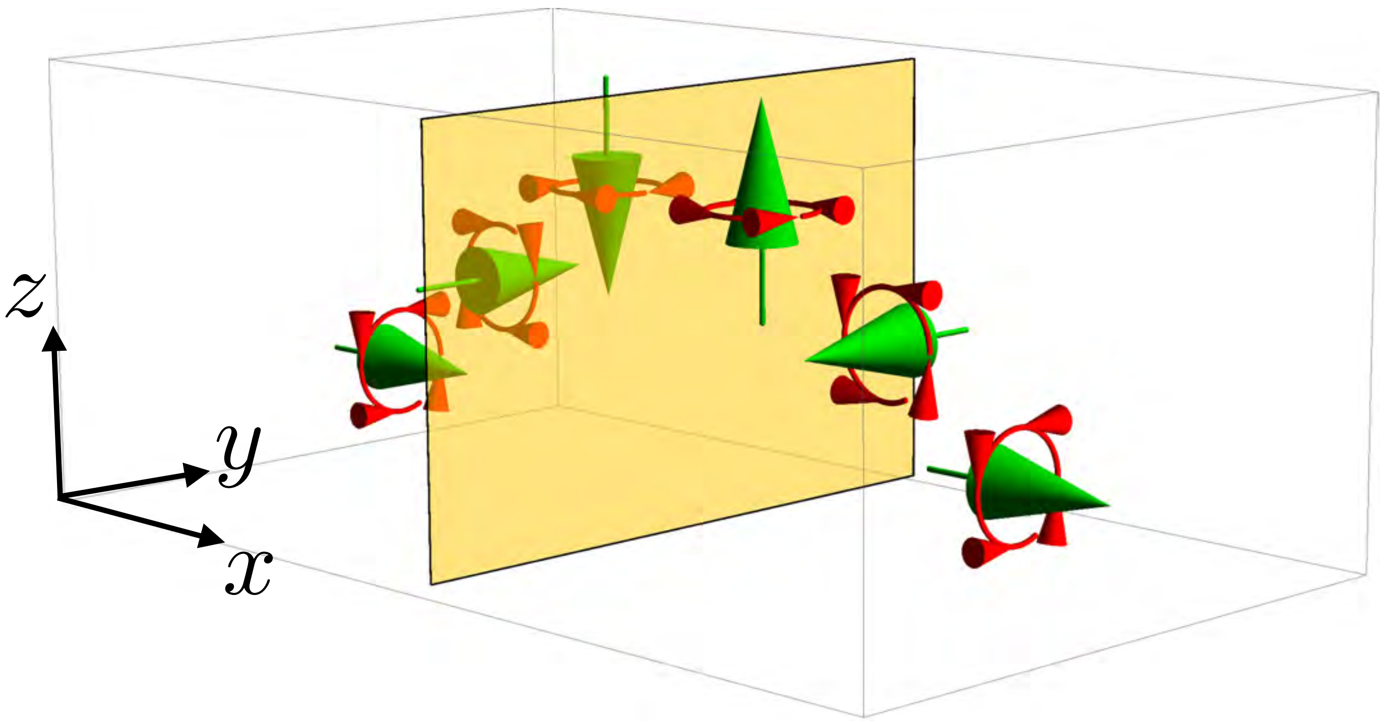
$|n_{\mathbb{Z}}| = \#$ gapless edge states (or surface states)

Reflection symmetry

- Consider reflection R: $x \rightarrow -x$

$$R^{-1}\mathcal{H}(-k_x,k_y,k_z)R = \mathcal{H}(k_x,k_y,k_z)$$

with $R = s_x$



— w.l.o.g.: eigenvalues of $R \in \{-1,+1\}$

Teo, Fu, Kane PRB '08

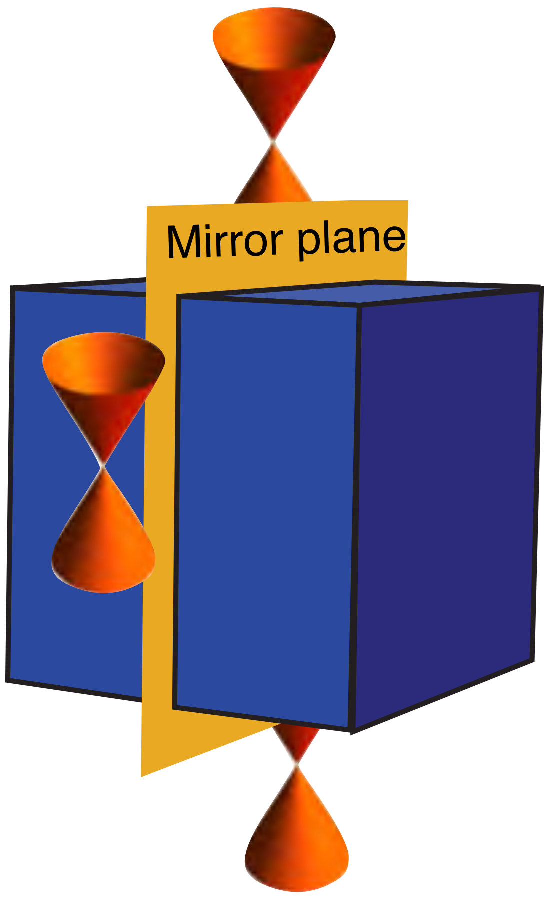
- **mirror Chern number:**

$$k_x = 0 \implies \mathcal{H}(0,k_y,k_z)R - R\mathcal{H}(0,k_y,k_z) = 0$$

— project $\mathcal{H}(0,k_y,k_z)$ onto eigenspaces of R: $\mathcal{H}_\pm(k_y,k_z)$

$$n_{\mathcal{M}}^{\pm} = \frac{1}{4\pi}\int_{\text{2D BZ}} \mathcal{F}_\pm \, d^2\mathbf{k}$$

Berry curvature in $\pm$ eigenspace



— total Chern number: $n_{\mathcal{M}} = n_{\mathcal{M}}^{+} + n_{\mathcal{M}}^{-}$

— mirror Chern number: $n_{\mathcal{M}} = n_{\mathcal{M}}^{+} - n_{\mathcal{M}}^{-}$

- Bulk-boundary correspondence:

— zero-energy states on surfaces that are left invariant under the mirror symmetry

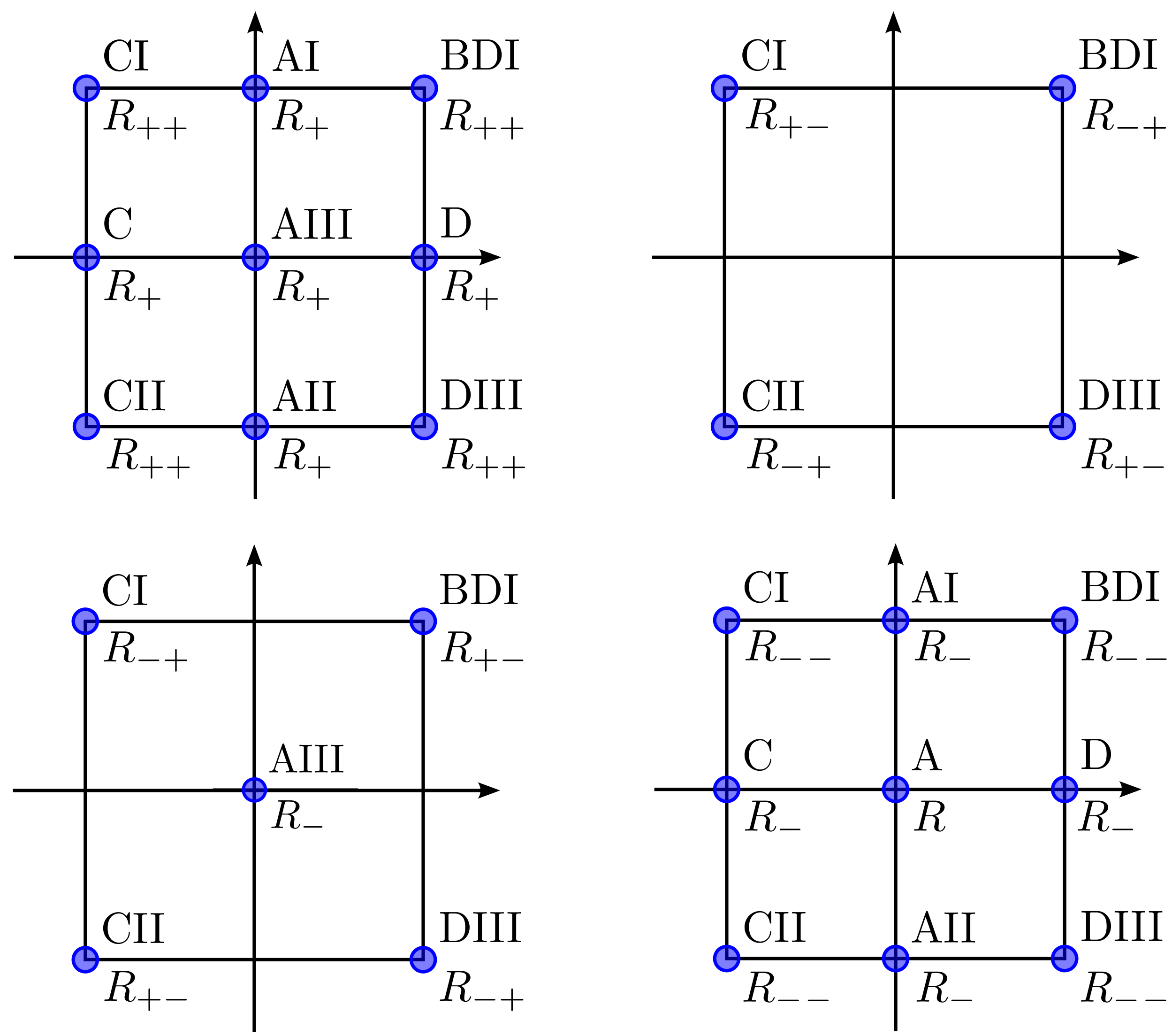
Classification of topological materials with reflection symmetry

R_+ : R commutes with T (C or S)

R_- : R anti-commutes with T (C or S)

Reflection	sym. class
R	A
R_+	AIII
R_-	AIII
R_+,R_{++}	AI
	BDI
	D
	DIII
	AII
	CII
	C
	CI
R_-,R_{--}	AI
	BDI
	D
	DIII
	AII
	CII
	C
	CI
R_{-+}	BDI, CII
R_{+-}	DIII, CI
R_{+-}	BDI
R_{-+}	DIII
R_{+-}	CII
R_{-+}	CI

"Bott cube"



Morimoto, Furusaki PRB 2013; Chiu, Schnyder PRB 2014;

Classification of topological materials with reflection symmetry

R_+ : R commutes with T (C or S) R_- : R anti-commutes with T (C or S)

Reflection	TI/TSC
	FS1
	FS2
R	A
R_+	AIII
R_-	AIII
	AI
	BDI
	D
R_+,R_{++}	DIII
	AII
	CII
	C
	CI
	AI
	BDI
	D
R_-,R_{--}	DIII
	AII
	CII
	C
	CI
R_{-+}	BDI, CII
R_{+-}	DIII, CI
R_{+-}	BDI
R_{-+}	DIII
R_{+-}	CII
R_{-+}	CI

?

For which symmetry class and dimension is there a topological insulator or topological semi-metal protected by reflection symmetry?

Classification of topological materials with reflection symmetry

R_+ : R commutes with T (C or S) R_- : R anti-commutes with T (C or S)

Reflection	TI/TSC	$d{=}1$	$d{=}2$	$d{=}3$	$d{=}4$	$d{=}5$	$d{=}6$	$d{=}7$	$d{=}8$
	FS1	$p{=}8$	$p{=}1$	$p{=}2$	$p{=}3$	$p{=}4$	$p{=}5$	$p{=}6$	$p{=}7$
	FS2	$p{=}2$	$p{=}3$	$p{=}4$	$p{=}5$	$p{=}6$	$p{=}7$	$p{=}8$	$p{=}1$
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0
R_+,R_{++}	AI	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$
	D	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	AII	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CII	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
	C	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CI	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
R_-,R_{--}	AI	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	BDI	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	D	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$
	AII	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	C	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CI	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
R_{-+}	BDI, CII	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
R_{+-}	DIII, CI	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0
R_{+-}	BDI	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$
R_{-+}	DIII	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0
R_{+-}	CII	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
R_{-+}	CI	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0

Chiu, Schnyder
PRB 2014

Classification of topological materials with reflection symmetry

R_+ : R commutes with T (C or S) R_- : R anti-commutes with T (C or S)

Reflection	TI/TSC	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
	FS1	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
	FS2	p=2	p=3	p=4	p=5	p=6	p=7	p=8	p=1
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	[illegible]	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0
R_+,R_{++}	AI	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	[illegible]	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$
	D	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	AII	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CII	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
	C	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CI	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
R_-,R_{--}	AI	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	BDI	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	D	$M\mathbb{Z}$	0	0	0	[illegible]	[illegible]	$T\mathbb{Z}_2$	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$
	AII	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	C	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CI	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
R_{-+}	BDI, CII	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
R_{+-}	DIII, CI	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0
R_{+-}	BDI	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$
R_{-+}	DIII	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus2\mathbb{Z}$	0
R_{+-}	CII	$2M\mathbb{Z}\oplus2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
R_{-+}	CI	0	0	$2M\mathbb{Z}\oplus2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0

Ca_3P_2

$CePt_3Si$

Ca_3PbO, Sr_3PbO

Chiu, Schnyder
PRB 2014

1. Topological insulators with reflection symmetry

Y. Nohara (MPI-FKF)

Yang-Hao Chan (A. Sinica)

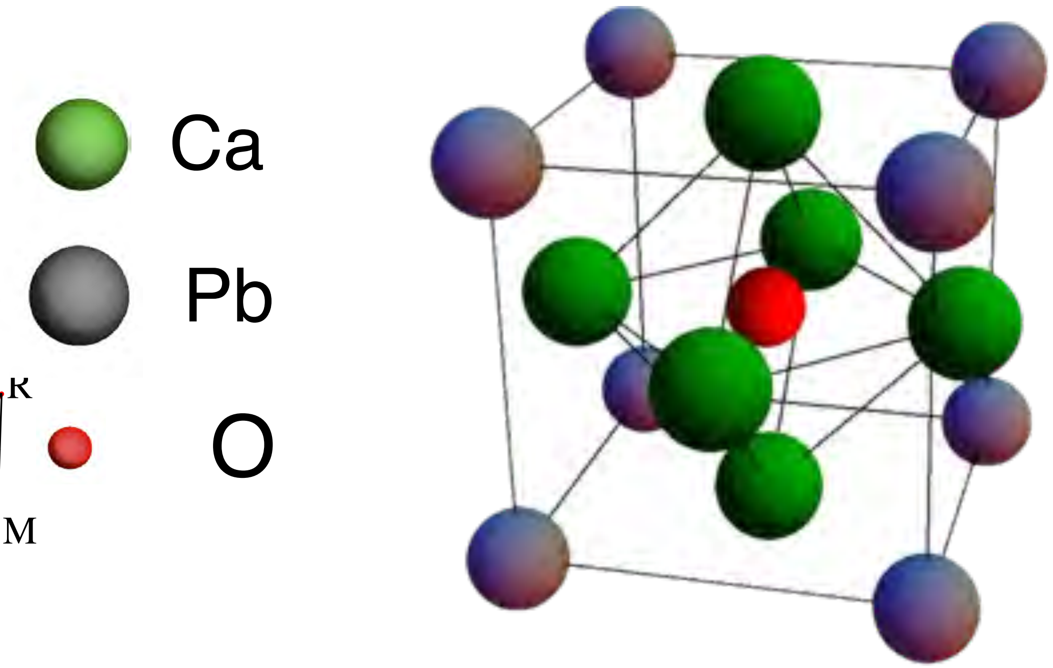
Ching-Kai Chiu (UMD)

Ca_3PbO, Sr_3PbO

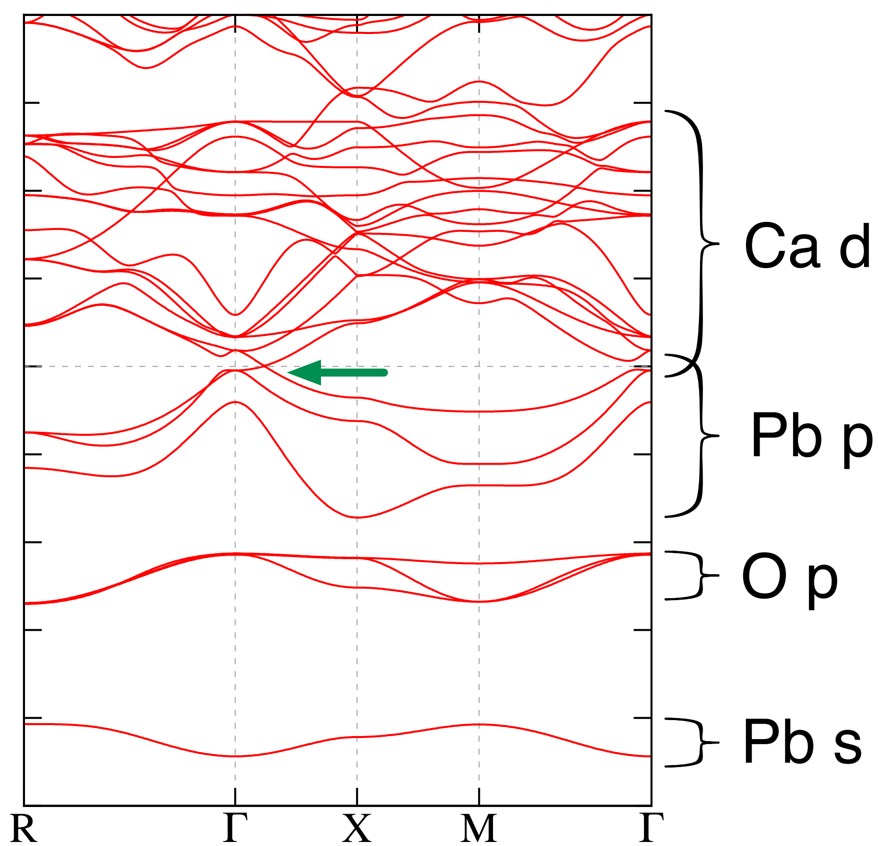
Ca$_3$PbO is a reflection symmetry protected TI

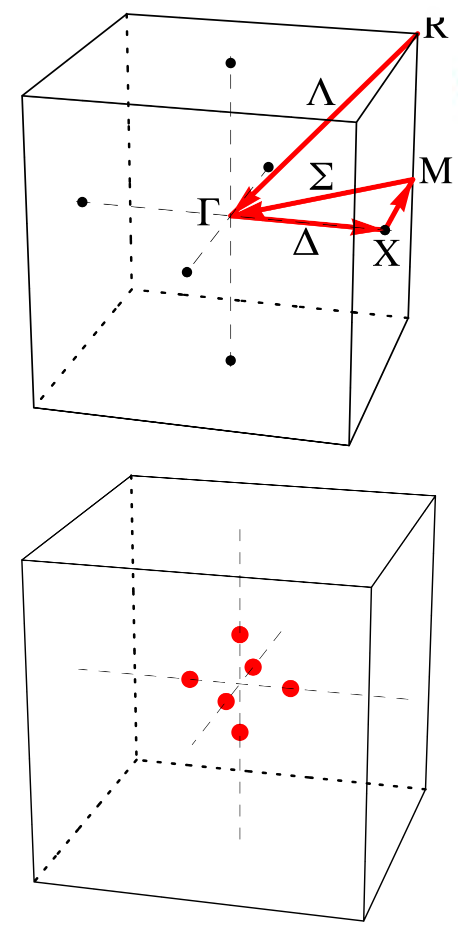
- Anti-perovskites: Ca$_3$PbO, Sr$_3$PbO

  in collaboration with A. Rost, H. Takagi



- Band structure (without SOC):





- Orbital character of bands:

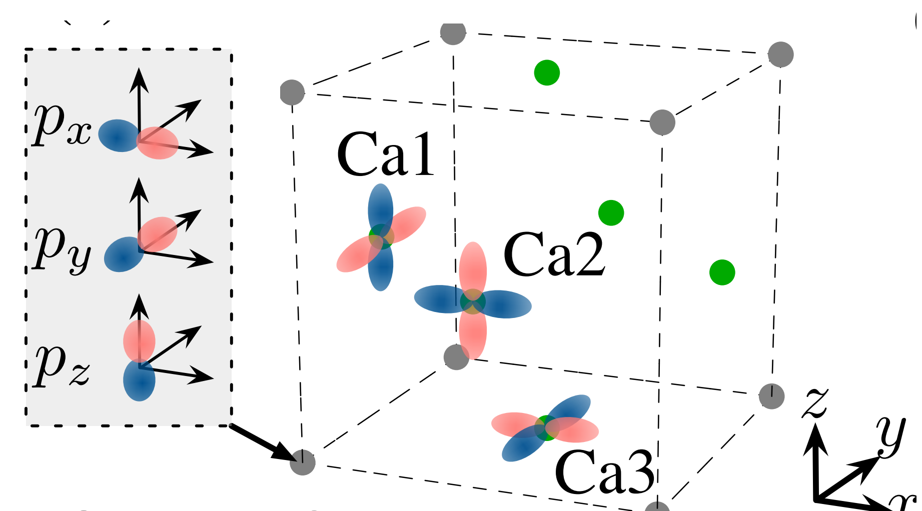
  Pb: $|p_x\rangle, |p_y\rangle, |p_z\rangle$

  Ca: $|d_{x^2-y^2}\rangle, |d_{x^2-z^2}\rangle, |d_{y^2-z^2}\rangle$

- Opening of bulk gap:

  hybridisation w/ Ca $|d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle$

  + SOC opens up bulk gap of ~10 meV



[after Kariyado and Ogata, JPSJ '12]

Ca_3PbO is a reflection symmetry protected TI

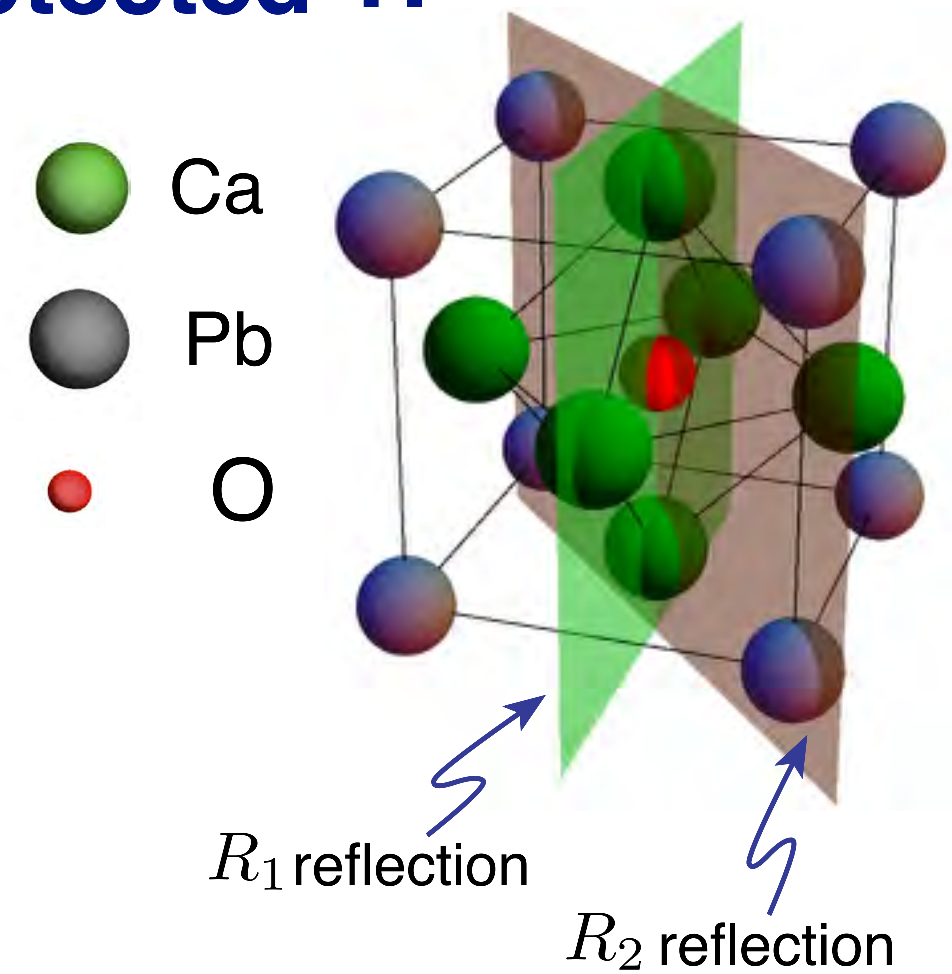
- Symmetries:

– Time-reversal: $T^{-1}\mathcal{H}(-\mathbf{k})T = +\mathcal{H}(\mathbf{k})$ $T = i s_y \mathcal{K}$

– two reflection symmetries : R_1 and R_2 R_-

R_j anti-commutes with T: $T R_j T^{-1} = -R_j$

$\Longrightarrow$ two mirror Chern numbers: $n_{\mathcal{M}_1}, n_{\mathcal{M}_2}$



Ca_3PbO is a reflection symmetry protected TI

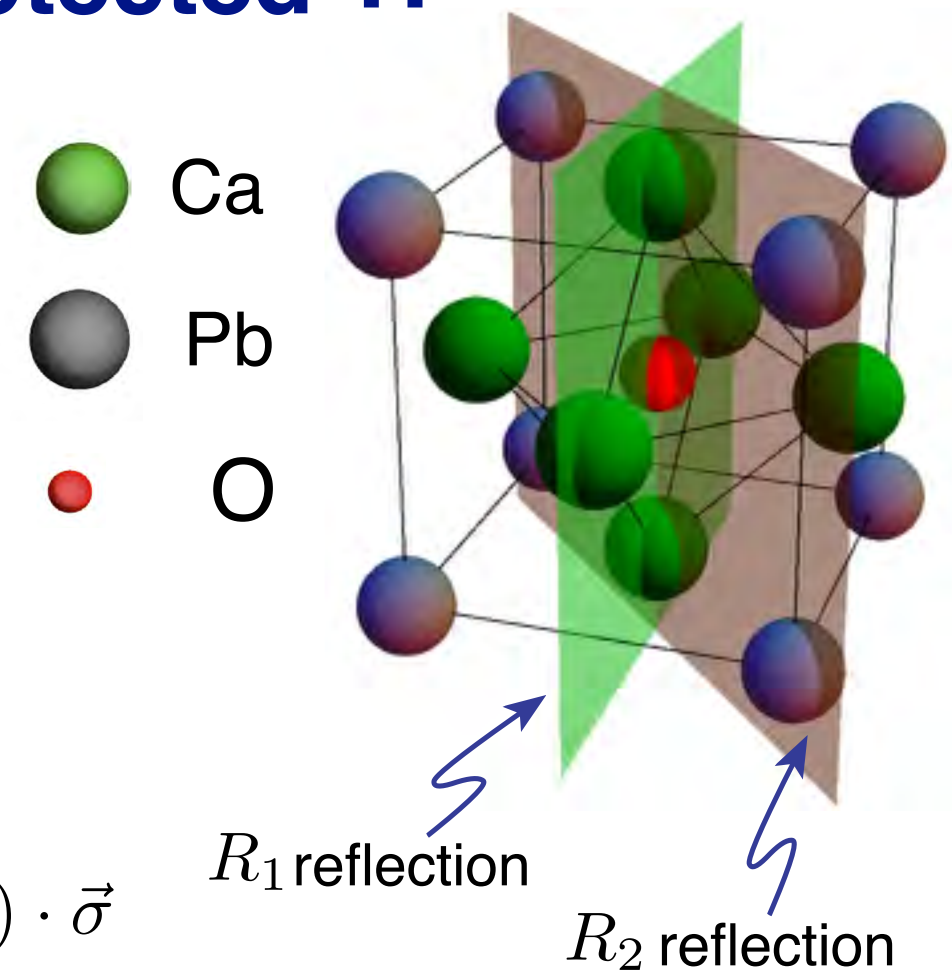
- Symmetries:

— Time-reversal: $T^{-1}\mathcal{H}(-\mathbf{k})T = +\mathcal{H}(\mathbf{k}) \quad T = is_y\mathcal{K}$

— two reflection symmetries : R_1 and R_2 $\quad R_-$

R_j anti-commutes with T: $TR_jT^{-1} = -R_j$

$\Longrightarrow$ two mirror Chern numbers: $n_{\mathcal{M}_1}, n_{\mathcal{M}_2}$



- Effective low-energy Hamiltonian for one Dirac cone within R_1 mirror plane:

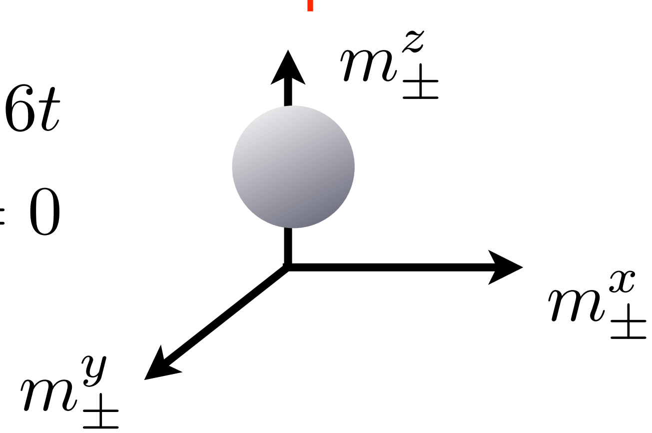
$$\mathcal{H}_\pm(k_y, k_z) = \pm \sin k_z \sigma_x \pm \sin k_y \sigma_y \pm \varepsilon_\mathbf{k} \sigma_z = \mathbf{m}_\pm(\mathbf{k}) \cdot \vec{\sigma}$$

$$E = \pm |\mathbf{m}_\pm(\mathbf{k})| \qquad \hat{\mathbf{m}}_\pm = \frac{\mathbf{m}_\pm(\mathbf{k})}{|\mathbf{m}_\pm(\mathbf{k})|}$$

trivial phase

$|\mu| > 6t$

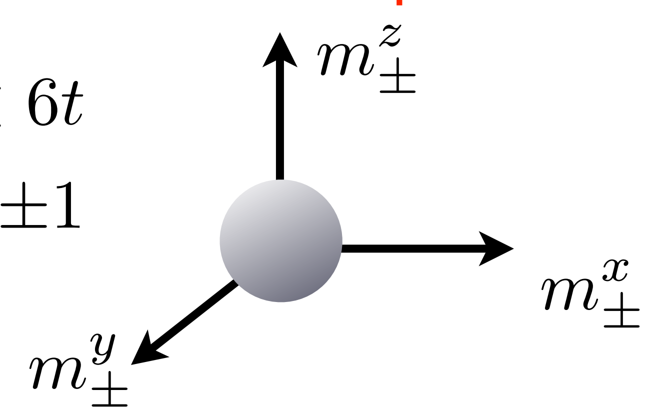
$n_\pm = 0$



non-trivial phase

$|\mu| < 6t$

$n_\pm = \pm 1$



$$\Longrightarrow n_\pm = \frac{1}{8\pi} \int_{\text{2D BZ}} d^2\mathbf{k}\, \epsilon^{\mu\nu} \hat{\mathbf{m}}_\pm \cdot \left[\partial_{k_\mu} \hat{\mathbf{m}}_\pm \times \partial_{k_\nu} \hat{\mathbf{m}}_\pm\right]$$

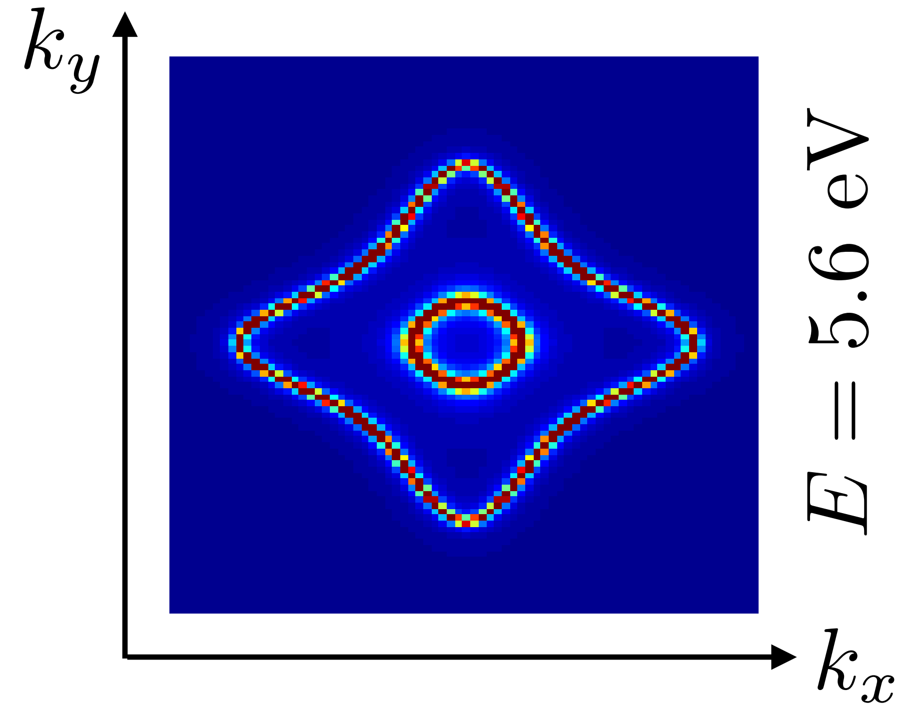
Ca_3PbO is a reflection symmetry protected TI

- Mirror Chern numbers:

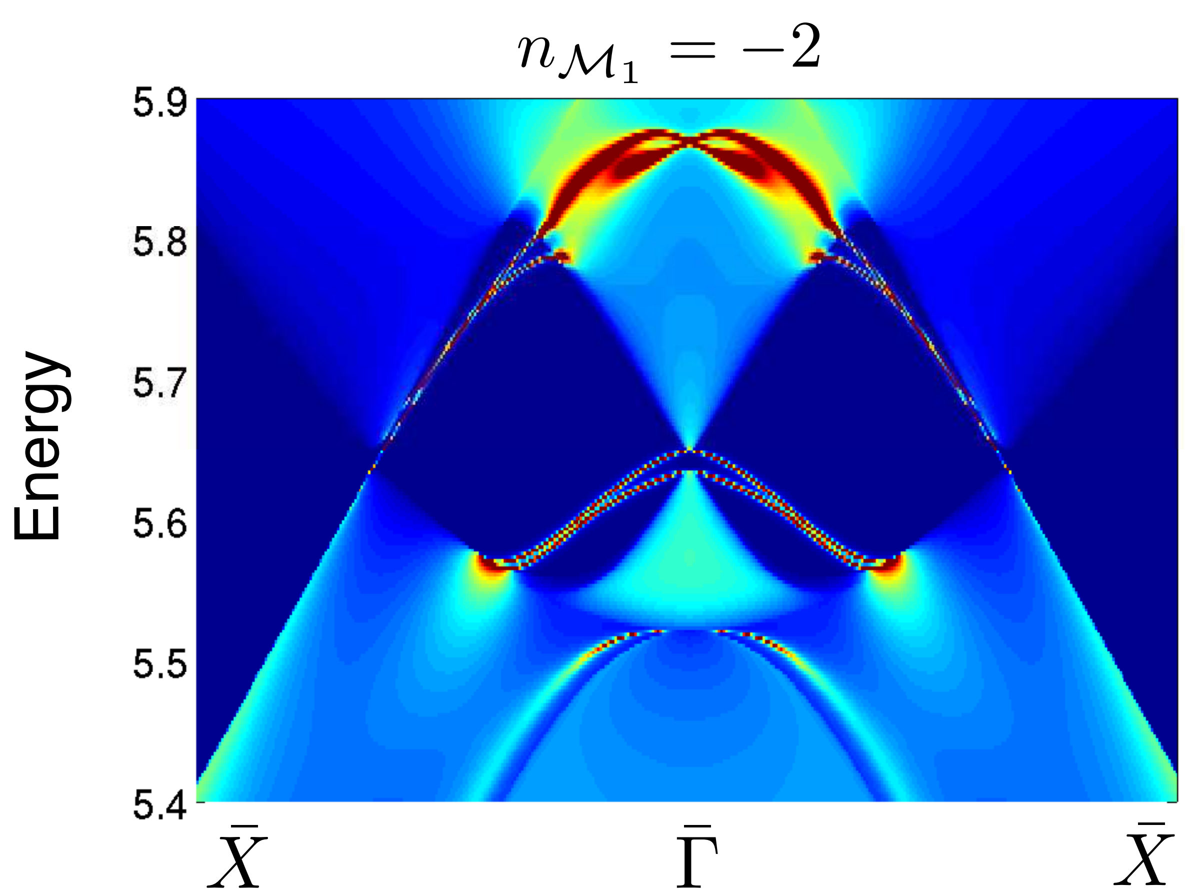
  – for Ca_3PbO: $n_{\mathcal{M}_1} = -2, \; n_{\mathcal{M}_2} = +2$

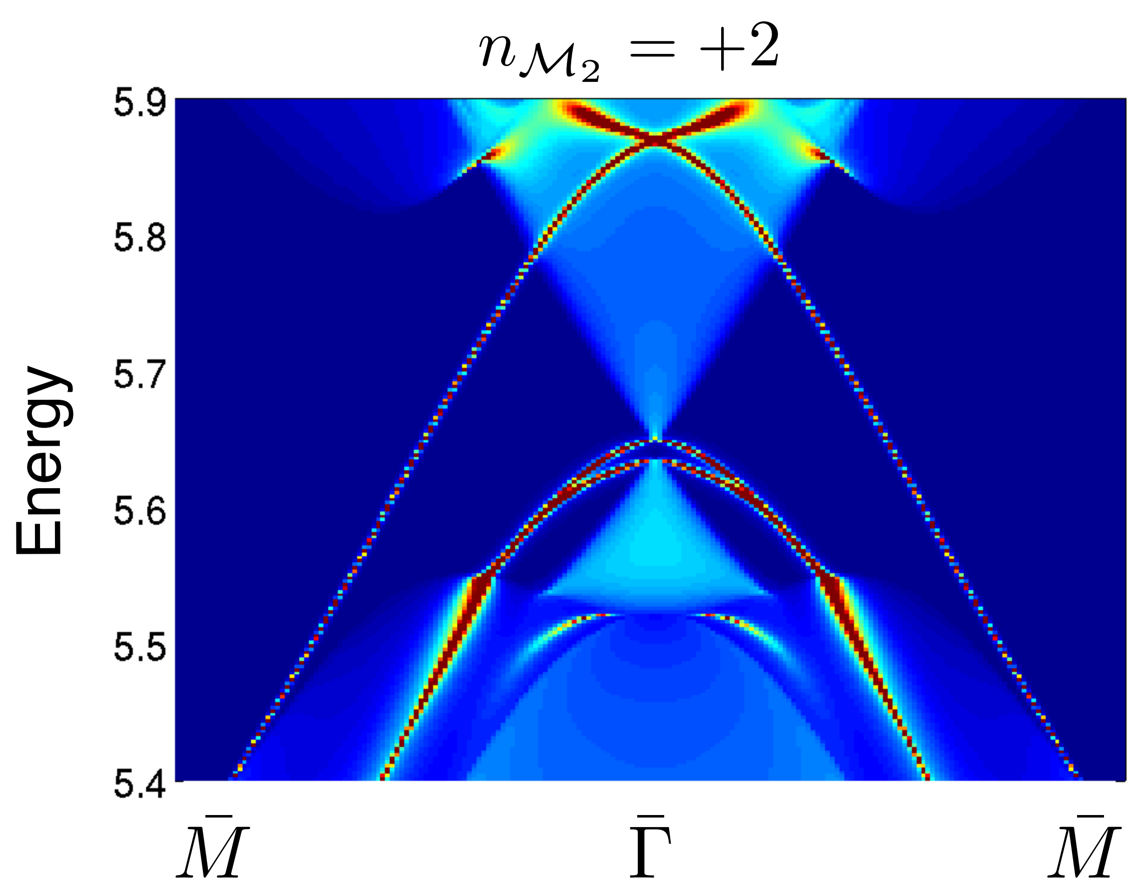
Bulk-boundary correspondence:

$|n_{\mathcal{M}}| = \#$ Dirac cone surface states



- Dirac cone surface states on (001) surface:





Chiu, Chan, Nohara, Schnyder, arXiv:1606.03456

Ca_3PbO is a reflection symmetry protected TI

- Type-II Dirac states on (111) surface:

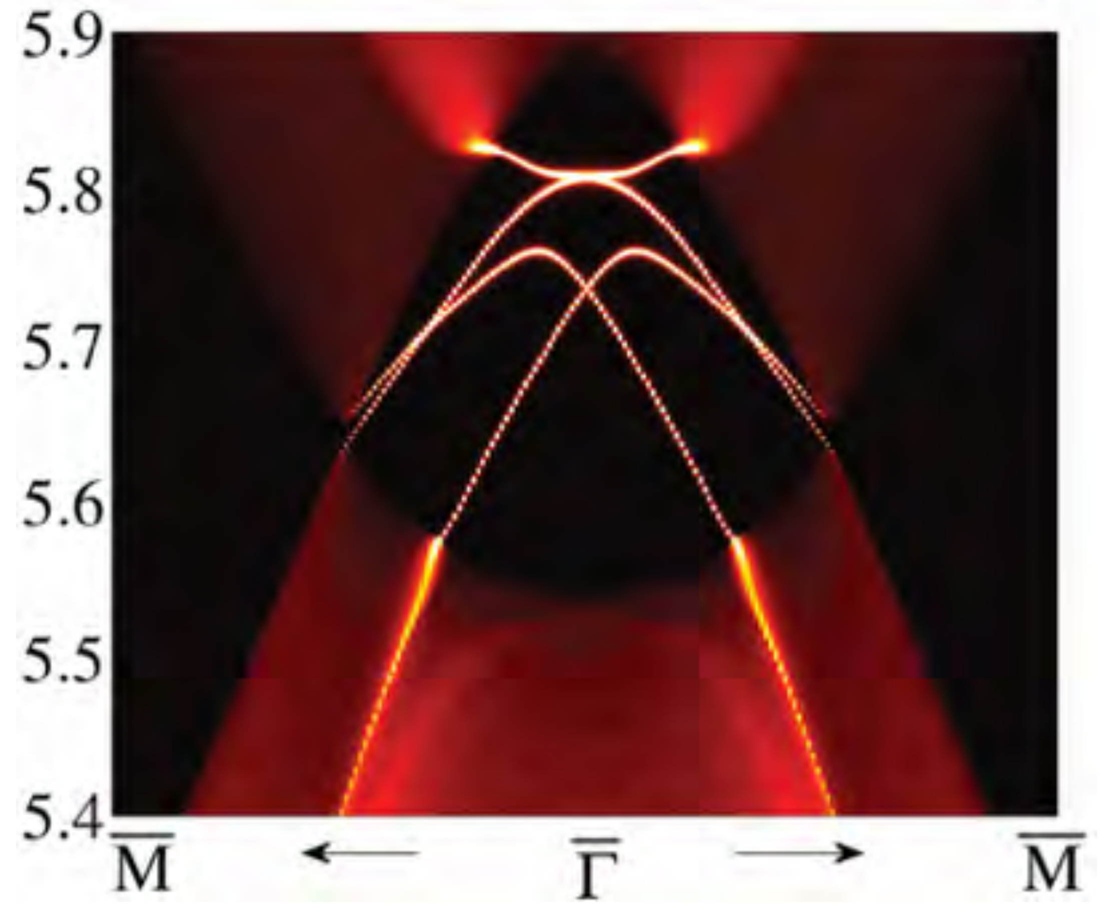
$$H^{\rm surf}_{\rm TCI}(k_x,k_y) = A k_y \sigma_0 + k_y \sigma_x - k_x \sigma_y$$

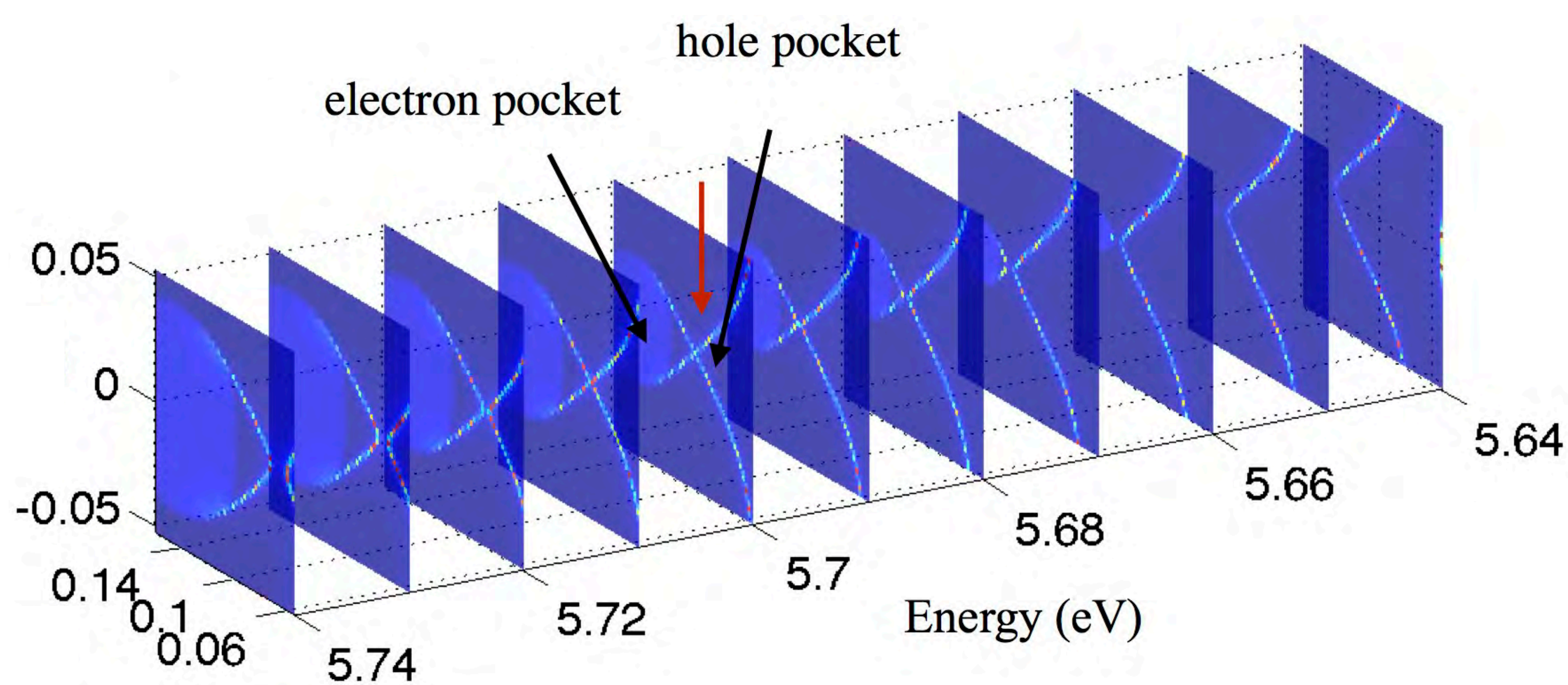
$$A > 0: \ \text{type-II Dirac state}$$

- Mirror symmetry: $R_x = \sigma_x$

$$R_x H^{\rm surf}_{\rm TCI}(-k_x,k_y) R_x^{-1} = H^{\rm surf}_{\rm TCI}(k_x,k_y)$$

- NB: $A k_y \sigma_0$ is forbidden by TRS



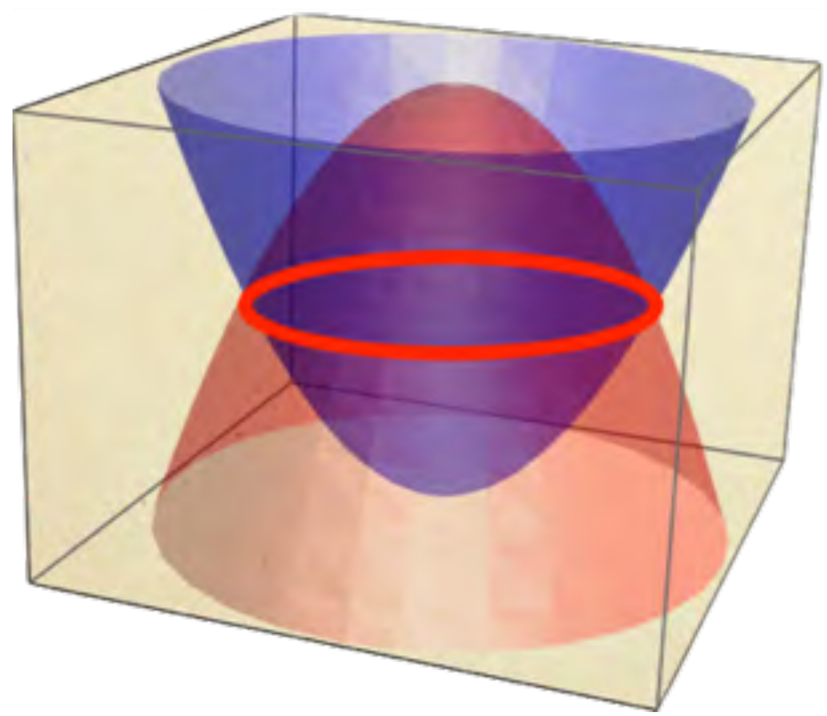


$\Rightarrow$ dense Landau level spectrum

Chiu, Chan, Nohara, Schnyder, arXiv:1606.03456

2. Topological nodal line semi-metals

Yang-Hao Chan (A. Sinica)



Ca_3P_2

Ching-Kai Chiu (UMD)

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R_+ : R commutes with T (C or S) R_- : R anti-commutes with T (C or S)

Reflection	TI/TSC	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
	FS1	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
	FS2	p=2	p=3	p=4	p=5	p=6	p=7	p=8	p=1
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	[illegible] $\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0
R_+,R_{++}	AI	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$
	D	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	AII	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CII	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
	C	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CI	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
R_-,R_{--}	AI	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	BDI	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	D	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$
	AII	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	C	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CI	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
R_{-+}	BDI, CII	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
R_{+-}	DIII, CI	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0
R_{+-}	BDI	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$
R_{-+}	DIII	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0
R_{+-}	CII	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
R_{-+}	CI	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0

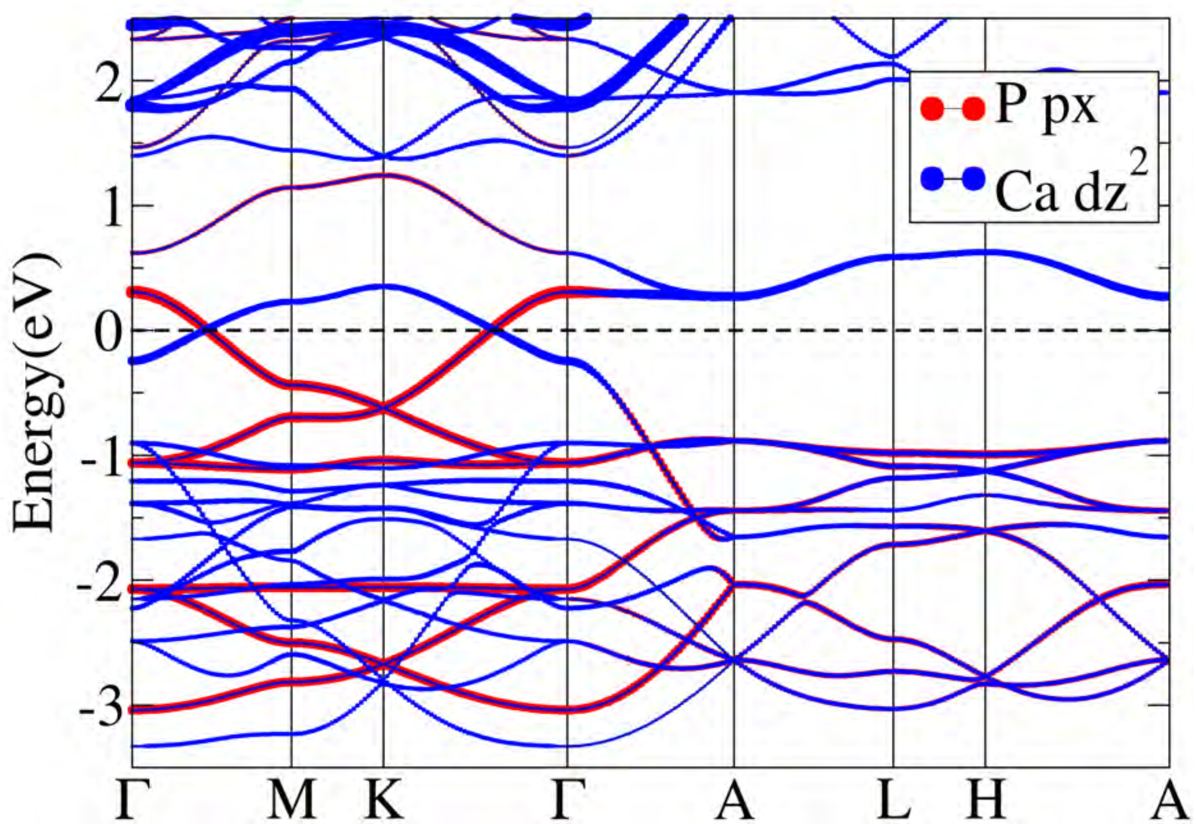
Ca_3P_2

Chiu, Schnyder
PRB 2014

Topological nodal lines in Ca_3P_2

see talk by Leslie Schoop

- Band structure:



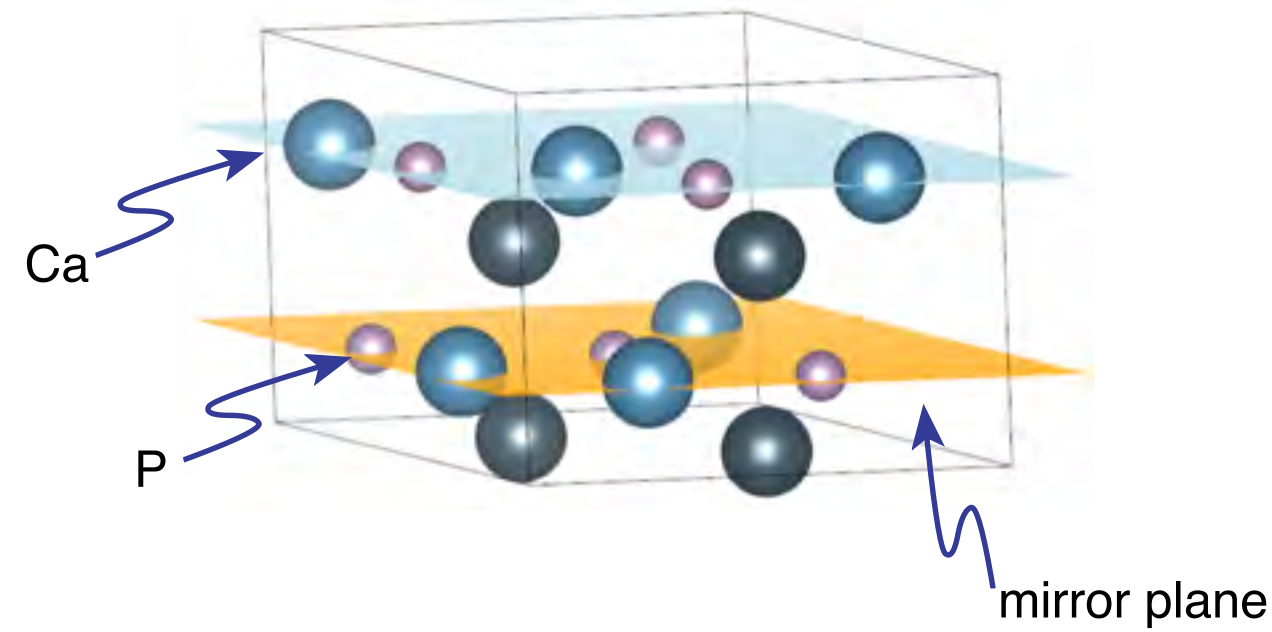
charge balanced: Ca^{2+} — P^{3-}

- Orbital character of bands near E_F:
  (6 Ca atoms, 6 P atoms)

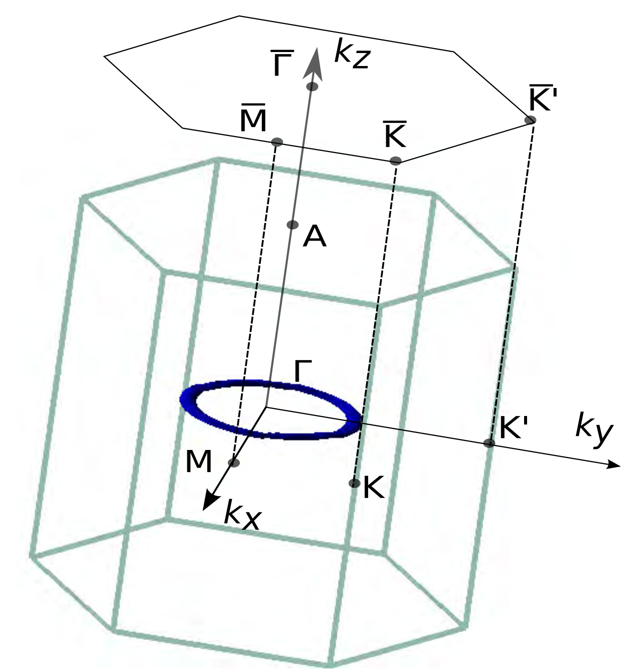
Ca: d_{z^2} orbitals from 6 Ca atoms

P: p_x orbitals from 6 P atoms

- Crystal structure $P6_3/mcm$



- Dirac ring within reflection plane



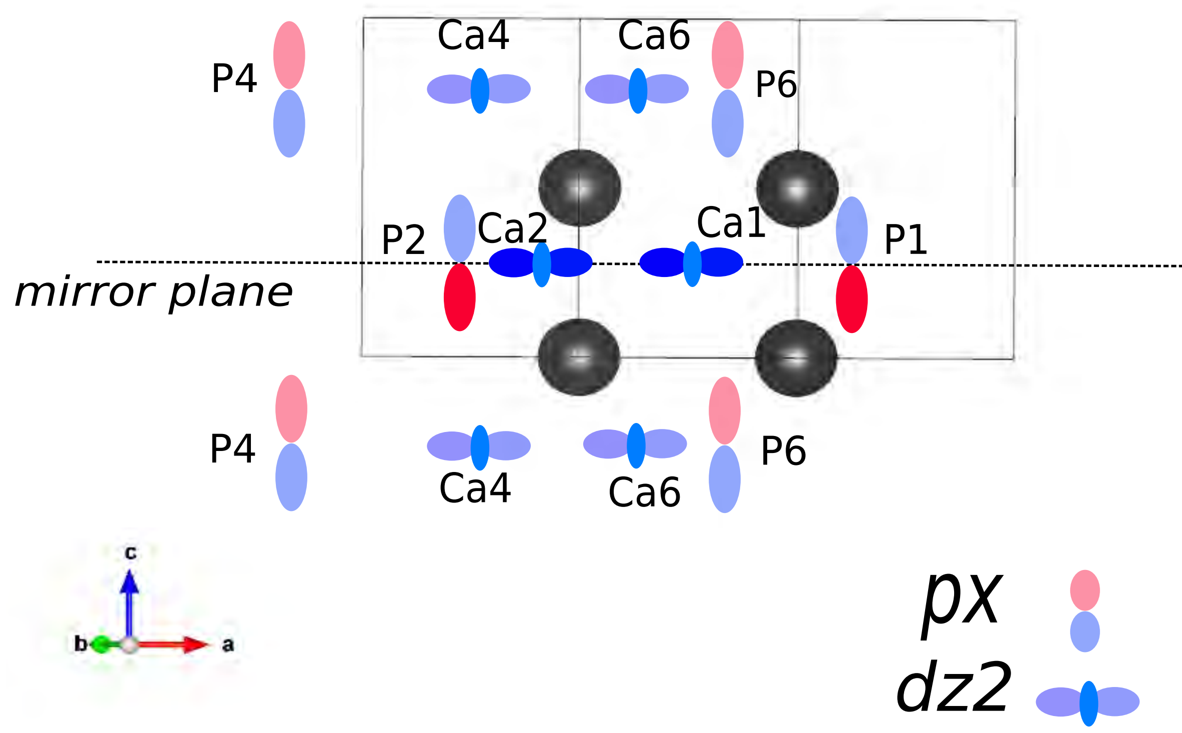
Chan, Chiu, Chou, Schnyder, Phys. Rev. B 93, 205132 (2016)

Topological nodal line: Mirror invariant

- **Reflection** $(z \to -z)$:

$$R^{-1}\mathcal{H}(k_x, k_y, -k_z)R = \mathcal{H}(k_x, k_y, k_z)$$

$$R(\mathbf{k}) = \begin{pmatrix} 1_{3\times3} & 0 & 0 & 0 \\ 0 & 1_{3\times3}e^{-ik_z} & 0 & 0 \\ 0 & 0 & -1_{3\times3} & 0 \\ 0 & 0 & 0 & -1_{3\times3}e^{-ik_z} \end{pmatrix}$$

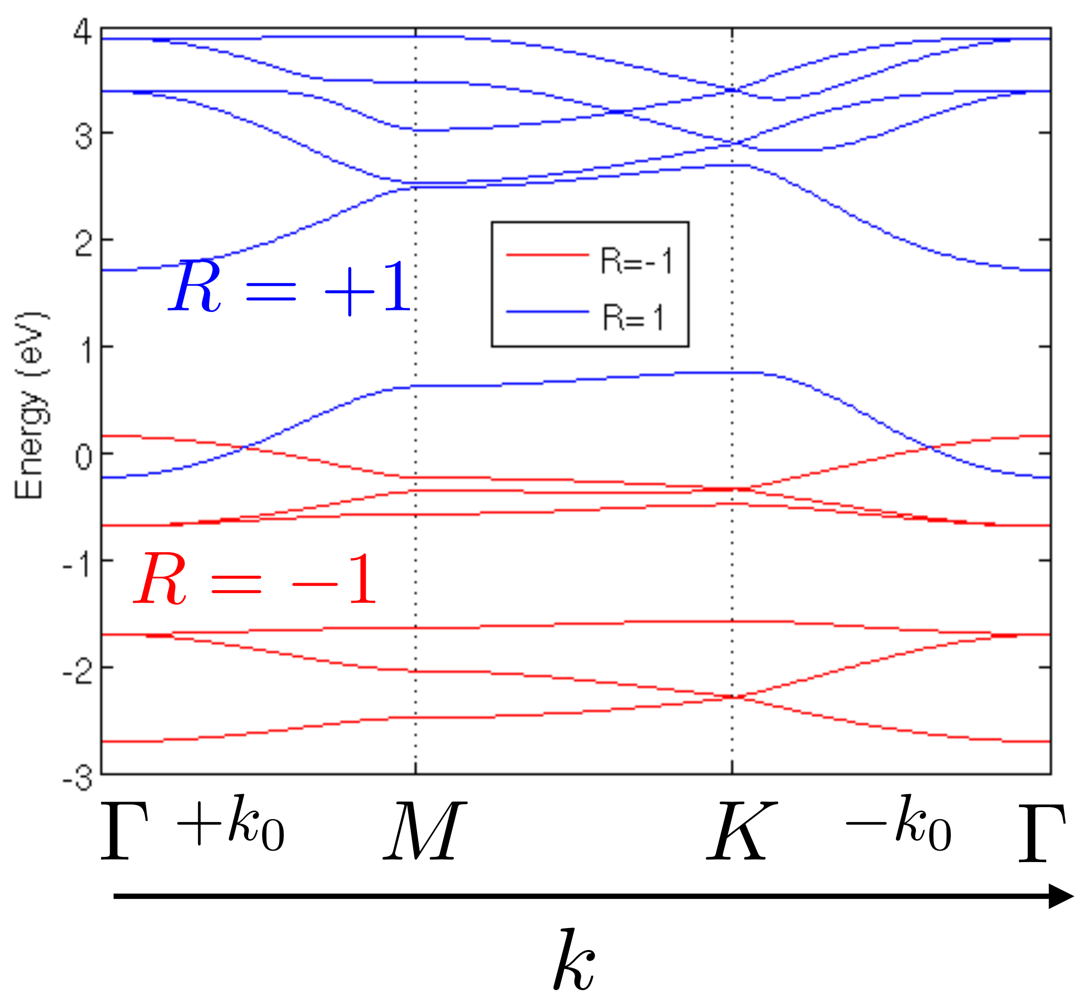


- **Mirror invariant:**

— number of occupied states with $R = +1$

$$N^0_{M\mathbb{Z}} = n^{+,0}_{\rm occ}(|k| > k_0) - n^{+,0}_{\rm occ}(|k| < k_0)$$

$$n^{+,0}_{\rm occ}(k) = \begin{cases} 1 & |k| < k_0 \\ 0 & |k| > k_0 \end{cases}$$



Chan, Chiu, Chou, Schnyder, Phys. Rev. B 93, 205132 (2016)

Drumhead surface state and Berry phase

▶ **Berry phase & charge polarization:**

$$\mathcal{P}(k_{\|}) = -i \sum_{j \in \text{filled}} \int_{-\pi}^{\pi} \left\langle u_{k_\perp}^{(j)} \middle| \partial k_\perp \middle| u_{k_\perp}^{(j)} \right\rangle dk_\perp$$

– $\mathcal{P}(k_{\|})$ quantized to $\pi \Rightarrow$ stable line node

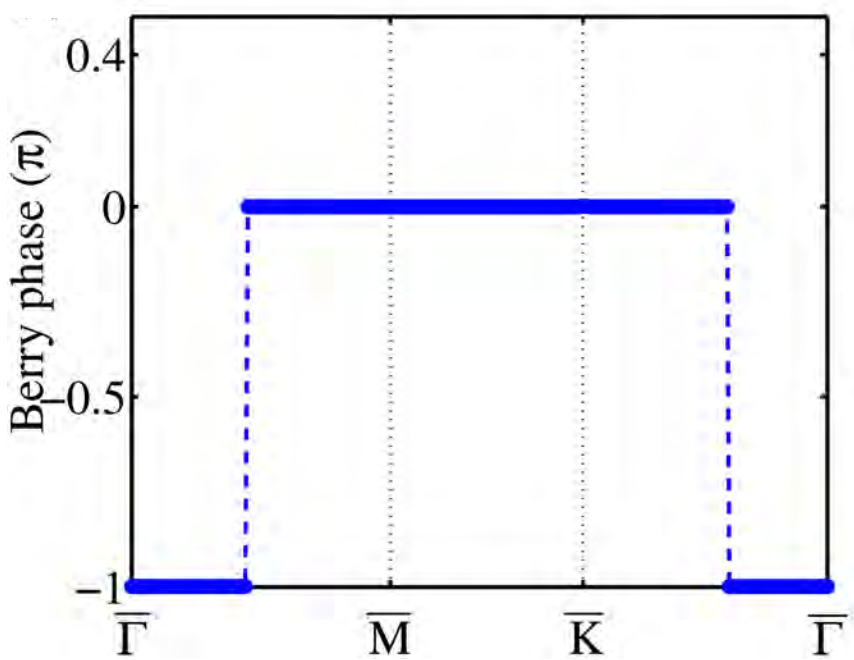
– In Ca_3P_2 Berry phase is quantized due to:

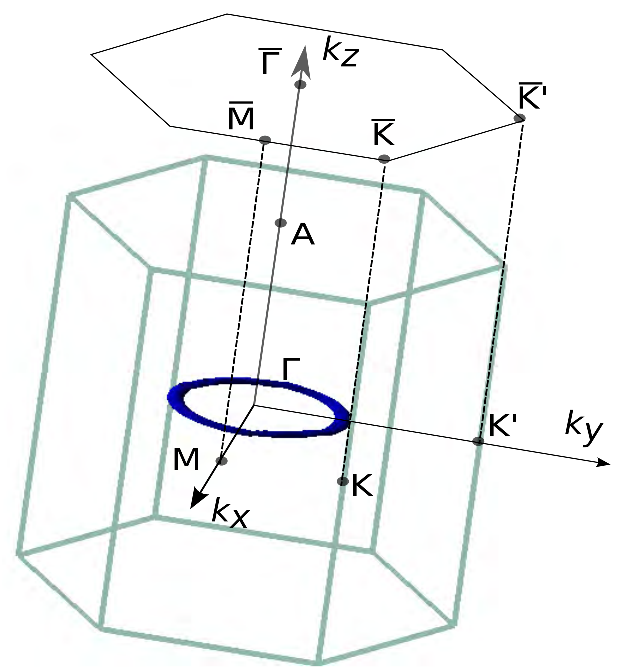
(i) reflection symmetry $z \to -z$

(ii) inversion + time-reversal symmetry

$$(-1)^{n_{\text{occ}}^{+,0}(k)+n_{\text{occ}}^{+,\pi}(k)} e^{i\partial R} = e^{i\mathcal{P}(k)}$$

Berry phase





Chan, Chiu, Chou, Schnyder, Phys. Rev. B 93, 205132 (2016)

Drumhead surface state and Berry phase

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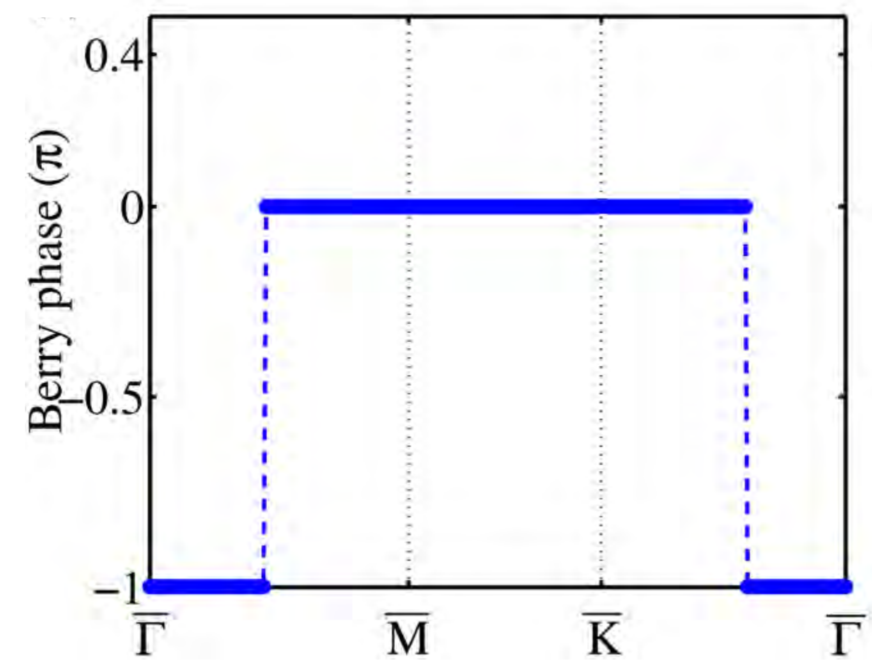
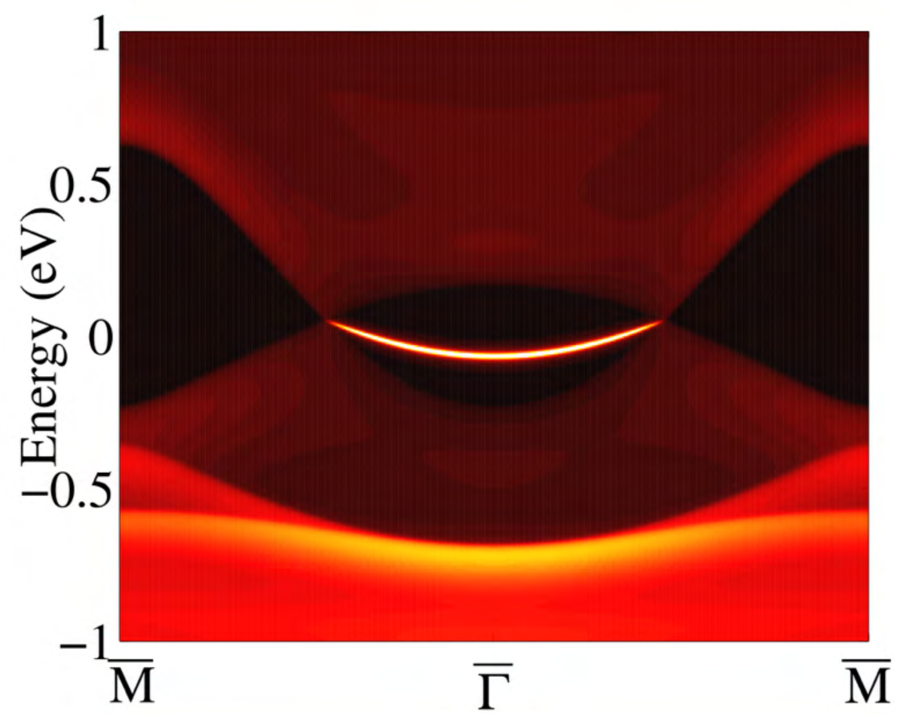
Berry phase



Surface spectrum



Bulk-boundary correspondence:

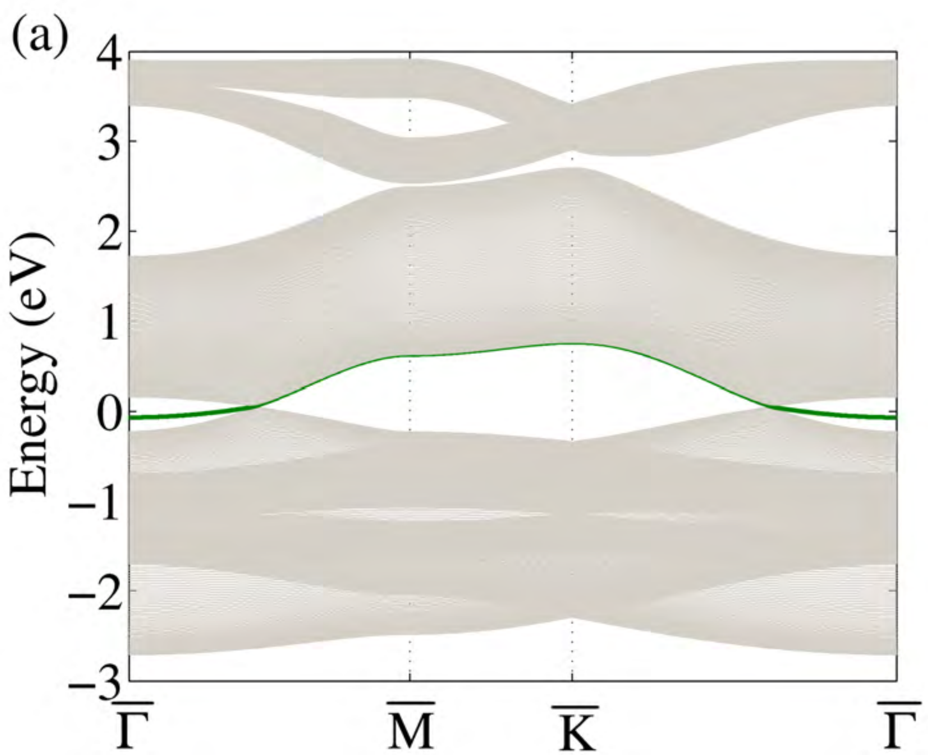
– surface charge: $\sigma_{\text{surf}} = \frac{e}{2\pi}\mathcal{P} \bmod e$

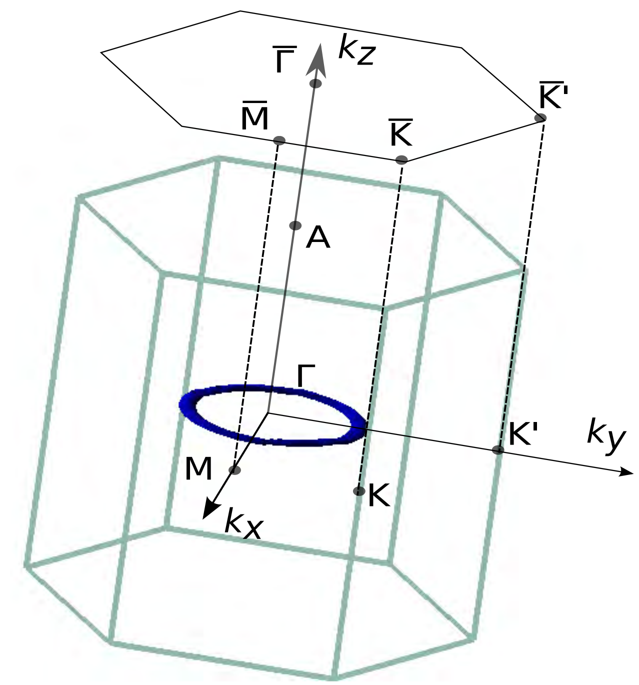
$\Rightarrow$ **Nearly flat 2D surface states connecting Dirac ring**

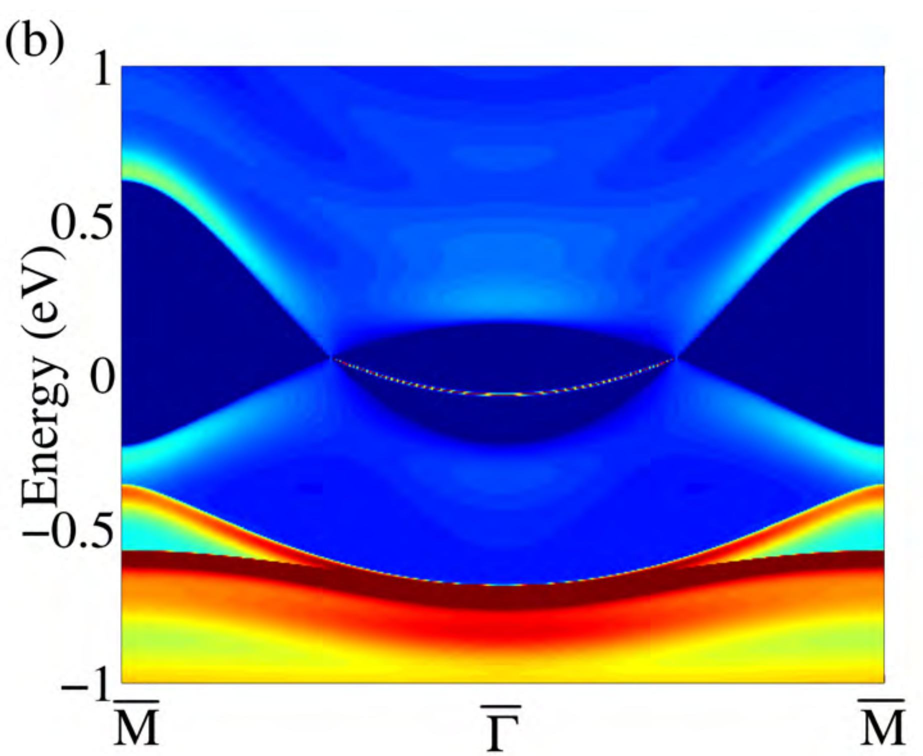
Chan, Chiu, Chou, Schnyder, Phys. Rev. B 93, 205132 (2016)

Drumhead surface state and Berry phase

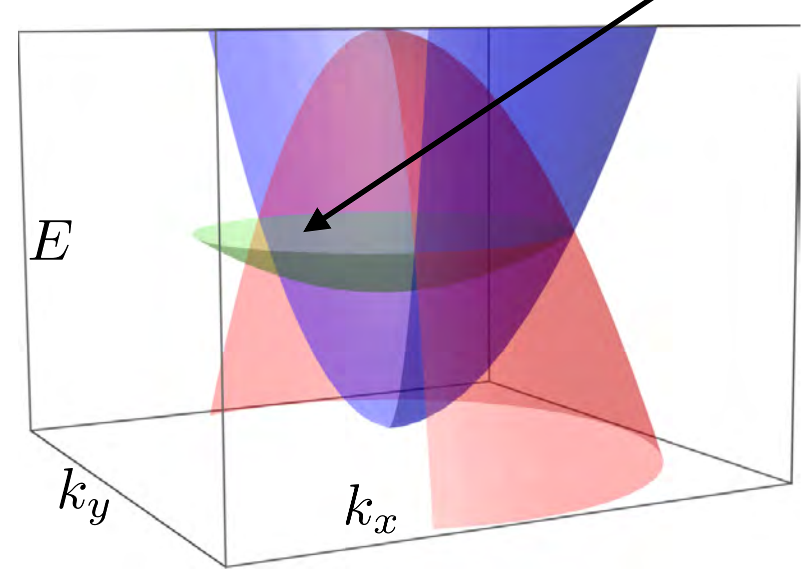
- **Nearly flat surface states connecting Dirac ring**





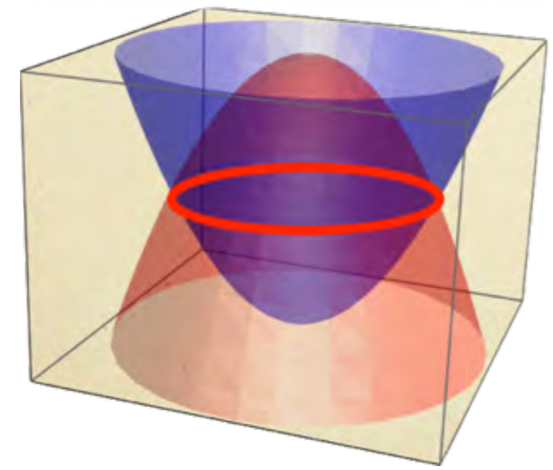


Drumhead surface state



Chan, Chiu, Chou, Schnyder, arXiv:1510.02759

Low-energy effective theory for Ca_3P_2



- low-energy effective Hamiltonian:

even in k

$$H_{\text{eff}}(\mathbf{k}) = (k_{\|}^2 - k_0^2)\tau_z + k_z\tau_y + f(\mathbf{k})\tau_0$$

- symmetry operators:

— reflection: $R = \tau_z$ — time-reversal: $T = \tau_0\mathcal{K}$ — inversion: $I = \tau_z$

- Gap-opening term τ_x is symmetry forbidden:

— breaks reflection symmetry: $R^{-1}\tau_x R = -\tau_x$

— breaks inversion + TRS: $(IT)^{-1}\tau_x IT = -\tau_x$

$\Rightarrow$ nodal line is stable

- $\mathbb{Z}$ versus $\mathbb{Z}_2$ classification:

$$H_{\text{eff}}(\mathbf{k}) \otimes \sigma_0 = (k_{\|}^2 - k_0^2)\tau_z \otimes \sigma_0 + k_z\tau_y \otimes \sigma_0 + f(\mathbf{k})\tau_0 \otimes \sigma_0$$

— consider gap opening term $\hat{m} = \tau_x \otimes \sigma_y$:

- (IT)-symmetric:

$$(\tau_z \otimes \sigma_0\mathcal{K})^{-1}\hat{m}(\tau_z \otimes \sigma_0\mathcal{K}) = \hat{m} \qquad \Rightarrow \mathbb{Z}_2 \text{ classification}$$

- but breaks R:

$$(\tau_z \otimes \sigma_0)^{-1}\hat{m}(\tau_z \otimes \sigma_0) \neq \hat{m} \qquad \Rightarrow \mathbb{Z} \text{ classification}$$

3. Nodal non-centrosymmetric superconductors

R. Queiroz (MPI-FKF)

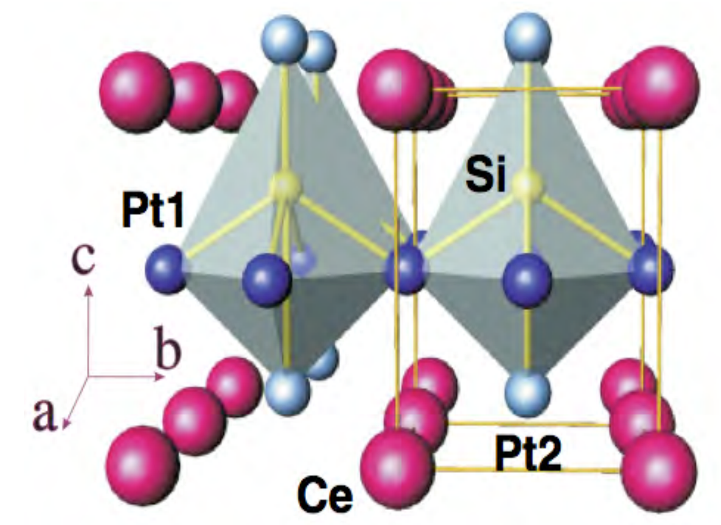
C. Timm (TU Dresden)

P. Brydon (U Otago)

$CePt_3Si$

Nodal non-centrosymmetric superconductors

[E. Bauer et al. PRL '04]



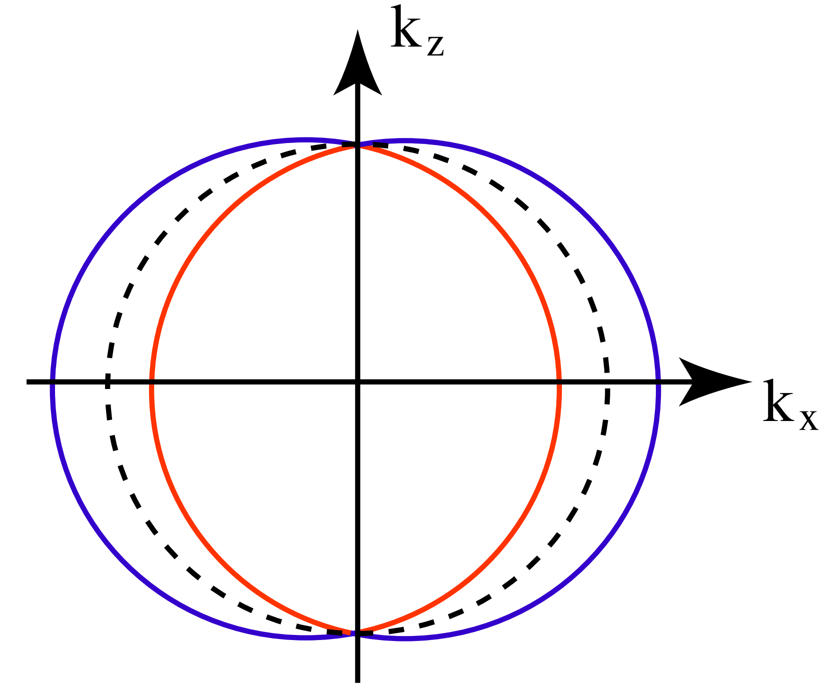
- Lack of inversion causes anti-symmetric SO coupling:

  Normal state: $\mathcal{H} = \sum_{\mathbf{k}} \Psi^{\dagger}_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} \sigma_0 + |\mathbf{g}_{\mathbf{k}}| \, \sigma_3 \right) \Psi_{\mathbf{k}}$

  SO coupling for C_{4v} point group: $\boldsymbol{g}_{\boldsymbol{k}} = k_y \hat{\boldsymbol{x}} - k_x \hat{\boldsymbol{y}}$

- Lack of inversion allows for admixture of spin-singlet and spin-triplet pairing components

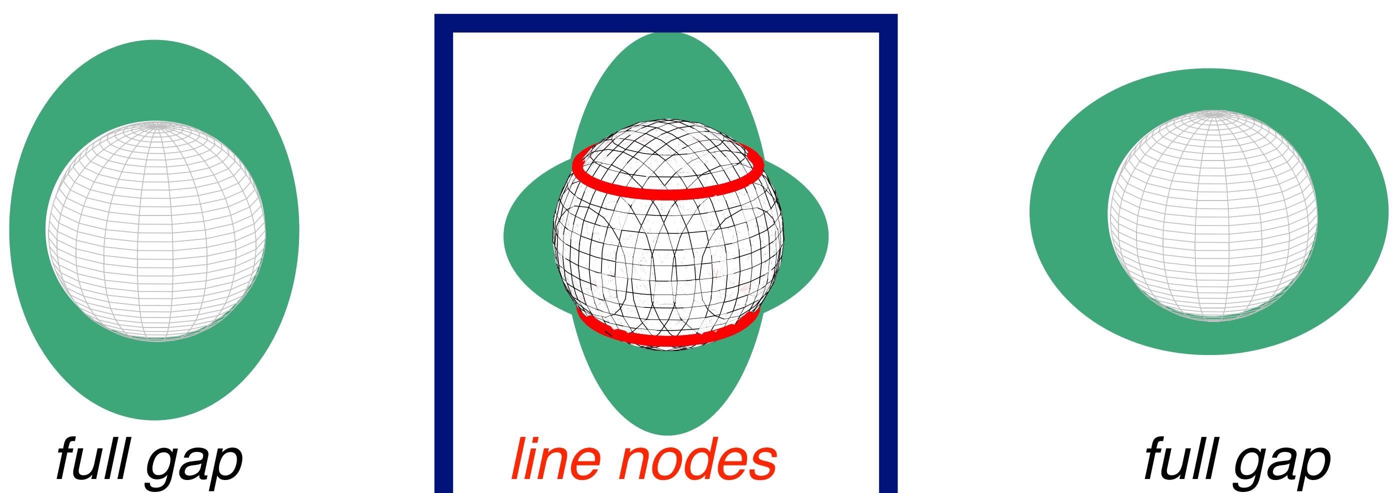
$$\Delta_{\mathbf{k}} = \left(\Delta_{\mathrm{s}} \sigma_0 + \Delta_{\mathrm{t}} \, \mathbf{d}_{\mathbf{k}} \cdot \vec{\sigma} \right) i \sigma_y \qquad (\boldsymbol{g}_{\boldsymbol{k}} \parallel \boldsymbol{d}_{\boldsymbol{k}})$$



Gaps on the two Fermi surfaces: $\Delta^{\pm}_{\boldsymbol{k}} = \Delta_s \pm \Delta_p \, |\boldsymbol{d}_{\boldsymbol{k}}|$

negative helicity FS

$\Delta_s > \Delta_t$ | $\Delta_s \sim \Delta_t$ | $\Delta_s < \Delta_t$

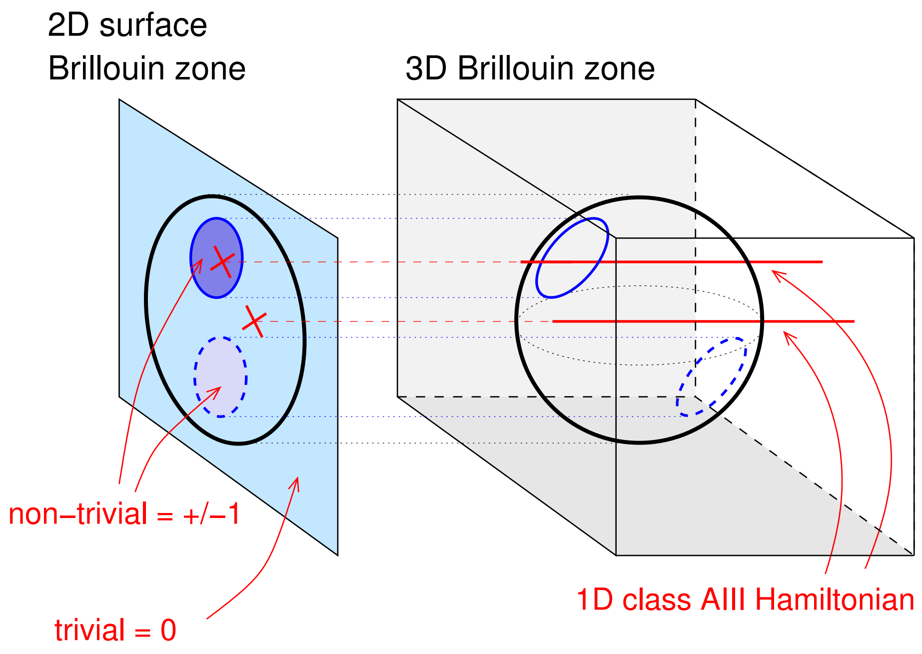


full gap | *line nodes* | *full gap*

Nodal non-centrosymmetric superconductors

- Symmetries: Time-reversal and particle-hole:

$$T = \sigma_0 \otimes i\sigma_2 \qquad T^2 = -1$$
$$C = \sigma_1 \otimes \sigma_0 \qquad C^2 = +1$$
$\Big\}$ class DIII



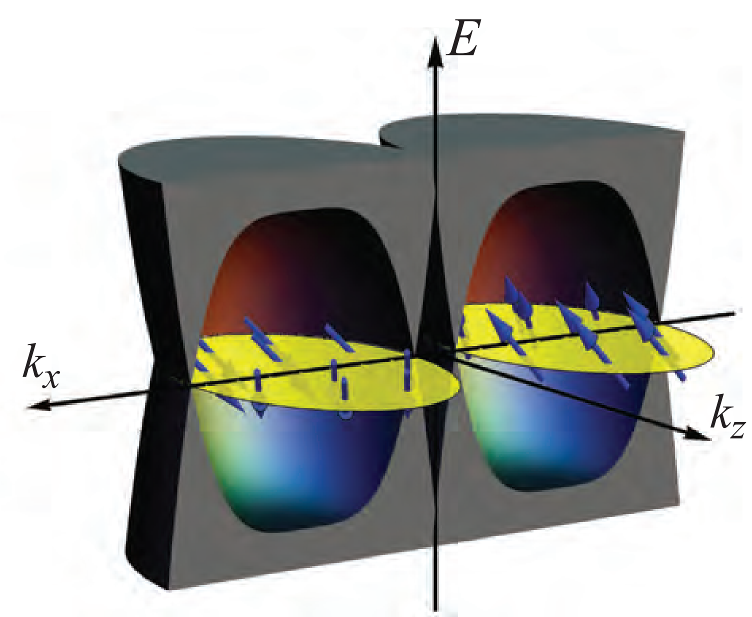
1D contour *in general* *not* centrosymmetric:

TRS ✗ PHS ✗ S=TRS x PHS ✓ $\Longrightarrow$ class AIII

- Winding number:

$$W_C = \frac{1}{2\pi} \oint_C dk_l \, \partial_{k_l} \left[\arg(\xi^-_{\mathbf{k}} + i\Delta^-_{\mathbf{k}}) \right]$$

$$\xi^\pm_{\mathbf{k}} = \varepsilon_{\mathbf{k}} \pm |\mathbf{g}_{\mathbf{k}}| \qquad \Delta^\pm_{\mathbf{k}} = \Delta_{\mathrm{s}} \pm \Delta_{\mathrm{t}} \, |\mathbf{d}_{\mathbf{k}}|$$



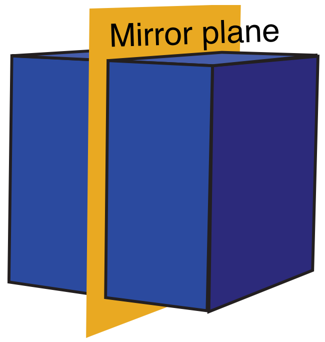
- Bulk-boundary correspondence:
  — surface flat bands

- Surface flat bands have Majorana character:

$$\gamma_k \sim \phi_{1,k}(r_\perp) \left(c_{k,\uparrow} - i\mathrm{sgn}(k) c^\dagger_{-k,\downarrow} \right) + \phi_{2,k}(r_\perp) \left(c_{k,\downarrow} + i\mathrm{sgn}(k) c^\dagger_{-k,\uparrow} \right)$$

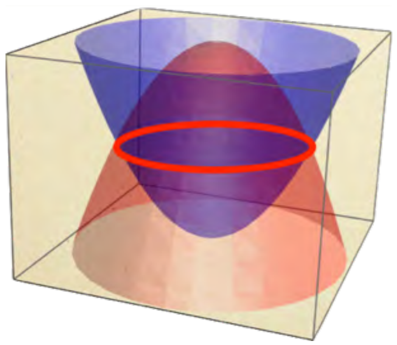
Schnyder, Ryu, PRB (2012)
Schnyder et al. PRL (2013)
Queiroz, Schnyder, PRB (2014)
Brydon et al. NJP (2015)
Queiroz, Schnyder, PRB (2015)

Conclusions and Outlook



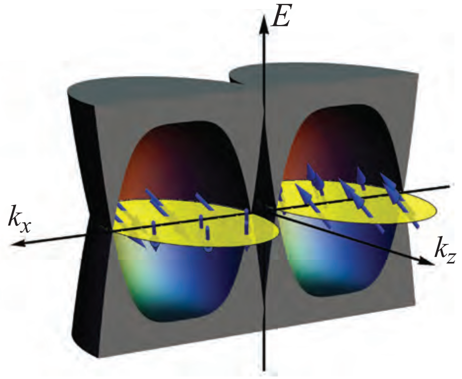
- Ca_3PbO is a topological insulator with reflection symmetry
  - Two Dirac surface states, type-II Dirac states

    arXiv:1606.03456



- Topological nodal line semi-metal Ca_3P_2
  - Drumhead surface states

    Phys. Rev. B 93, 205132 (2016)



- Nodal non-centrosymmetric superconductor $CePt_3Si$
  - Majorana flat band surface states

- Topological classification schemes:

  (i) bring order to the growing zoo of topological materials

  (ii) give guidance for the search and design of new topological states

  (iii) link the properties of the surface states to the bulk wave function topology

Review articles: arXiv:1505.03535; J. Phys.: Condens. Matter 27, 243201 (2015)